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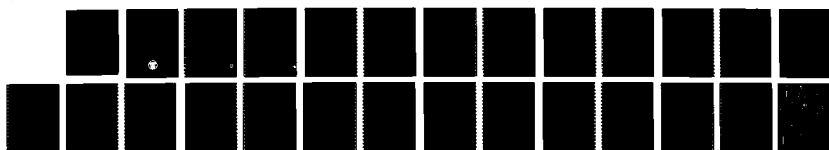
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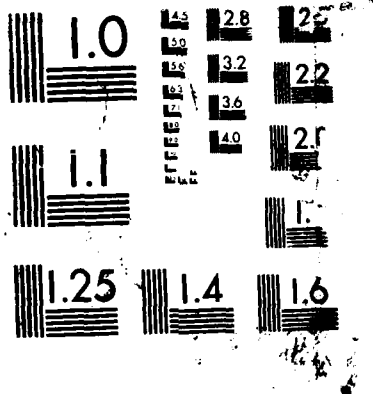
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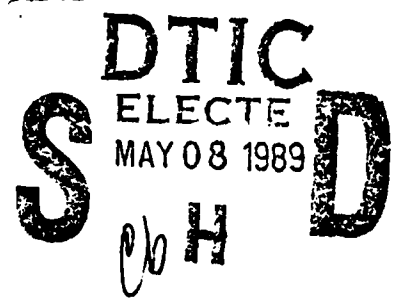
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On a Computational Method for the Second Fundamental Tensor
and its Application to Bifurcation Problems*

by

Werner C. Rheinboldt and Patrick J. Rabier

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* This work was in part supported by the National Science Foundation (DCR-8309926) and the Office of Naval Research (N-00014-80-C-9455). The second author began some of the work while visiting the University of Heidelberg/Germany as an Alexander von Humboldt Senior U. S. Scientist.

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On a Computational Method for the Second Fundamental Tensor
and its Application to Bifurcation Problems*

by
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and
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Dedicated to Professor Richard S. Varga on the occasion of his
60th birthday.

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Abstract: An algorithm is presented for the computation of the second fundamental tensor V of a Riemannian submanifold M of \mathbb{R}^n . From V the Riemann curvature tensor of M is easily obtained. Moreover, V has a close relation to the second derivative of certain functionals on M which, in turn, provides a powerful new tool for the computational determination of multiple bifurcation directions. Frequently, in applications, the manifold M is defined implicitly as the zero set of a submersion F on \mathbb{R}^n . In this case, the principal cost of algorithm for computing $V(p)$ at a given point $p \in M$ involves only the decomposition of the Jacobian $DF(p)$ of F at p and the projection of $d(d+1)$ neighboring points onto M by means of a local iterative process using $DF(p)$. Several numerical examples are given which show the efficiency and dependability of the method. *(1.8)*

1. Introduction

In recent years various computational methods for the analysis of differentiable manifolds have been developed, see e.g. [8],[9],[10] where also other references can be found. These methods have numerous applications in the study of multi-parameter equilibrium problems and their bifurcation behavior. But, up to now, there appear to exist no general purpose numerical methods for the computation of the curvature tensor of a Riemannian manifold M or any of its related quantities. Yet, the curvature tensor incorporates all the infor-

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mation about the metric properties of M and hence is of considerable importance in the solution of problems which intrinsically involve the metric of M .

In this paper we present a first algorithm for the computation of the second fundamental tensor of a sub-manifold M of R^n on which a Riemannian metric is induced by the Euclidean inner product on R^n . Our reason for concentrating on the second fundamental tensor is two-fold. First of all, this tensor retains all the information about the metric properties of the manifold, and the Riemann curvature tensor can be computed from it by means of a simple formula (see e.g. [12] and section 2 below). On the other hand, the second fundamental tensor has a close relationship with the second derivative of certain real valued functionals on the manifold and this, in turn, provides a powerful new tool for a computational analysis of non-degenerate bifurcation phenomena when possible multiple branching occurs.

In Section 2 below we summarize our notation and collect, without proof, some key results from Riemannian geometry. Full proofs can be found in most texts in this area, as, for instance, [1] or [12]. Section 3 introduces the concepts leading to the calculation of the second fundamental tensor, and then in Section 4 these concepts are used to formulate our principal algorithm. In Section 5 we discuss the indicated application of this algorithm to the computation of bifurcation directions. The algorithm has been implemented as a general purpose FORTRAN package which provides also an interface to the methods discussed in the mentioned earlier references [8]-[10] as well as to the continuation code PITCON (see [11]). Some experimental results with this package involving various bifurcation problems are presented in Section 6.

2. Basic concepts from Riemannian geometry.

We denote by $\bar{\nabla}$ the standard connection (covariant differentiation) in \mathbb{R}^n . In other words, for any smooth vector fields X and Y on \mathbb{R}^n , $\bar{\nabla}_X Y$ is the vector field obtained by differentiating Y in the direction X .

Throughout this paper, $M \subset \mathbb{R}^n$ will be a smooth sub-manifold with dimension $d \geq 2$. Then, for two vector fields X and Y that are tangent to M , $\bar{\nabla}_X Y$ is defined for any extension of X and Y to vector fields on \mathbb{R}^n . As a vector field on M (with values in \mathbb{R}^n), $\bar{\nabla}_X Y$ turns out to be independent of these extensions.

It will be assumed that \mathbb{R}^n is equipped with the canonical inner product $\langle \cdot, \cdot \rangle$ which induces the Riemannian metric on M . Accordingly, orthogonality will always be understood in the sense of this inner product. Then, for any vector fields X and Y tangent to M we have

$$\bar{\nabla}_X Y = \nabla_X Y + V(X, Y), \quad (2.1)$$

where $\nabla_X Y$ and $V(X, Y)$ are the tangential and normal components of $\bar{\nabla}_X Y$, respectively. In other words, for $p \in M$, $(\nabla_X Y)_p$ and $(V(X, Y))_p$ are the orthogonal projections of $(\bar{\nabla}_X Y)_p$ onto the tangent space $T_p M$ and the normal space $N_p M$ of M at p , respectively.

While the operator ∇ of (2.1) is a connection on M , it is well known that V is a symmetric vector-valued 2-covariant tensor, called the second fundamental tensor. In particular, the value $(V(X, Y))_p$ depends only on the values X_p and Y_p of the vector fields X and Y at p , and not on the field nature of X and Y .

As noted in the introduction, we are interested in the numerical evaluation of the second fundamental tensor V at a given point $p \in M$; that is, in

the computation of $V(X_p, Y_p)$ for an arbitrary pair of vectors X_p and Y_p that are tangent to M at p .

As observed before, the second fundamental tensor is closely connected with the Riemann curvature tensor R on M . In fact, for any four vector fields X, Y, Z, W tangent to M , the following simple formula holds

$$\langle R(X, Y)Z, W \rangle = \langle V(X, W), V(Y, Z) \rangle - \langle V(X, Z), V(Y, W) \rangle, \quad (2.2)$$

(see [12, Vol. IV, p. 47] and recall that the curvature tensor of R^n is zero).

In particular, for $W = X$ and $Z = Y$, it follows that

$$\langle R(X, Y)Y, X \rangle = \langle V(X, X), V(Y, Y) \rangle - |V(X, Y)|^2, \quad (2.3)$$

where $|\cdot|$ denotes the Euclidian norm. The relation (2.3), in turn, allows for the computation of the curvature $k(P)$ of any plane $P = \text{span}\{X_p, Y_p\} \subset T_p M$ since

$$k(P) = \frac{\langle R(X_p, Y_p)Y_p, X_p \rangle}{A(X_p, Y_p)} \quad (2.4)$$

where

$$A(X_p, Y_p) = |X_p|^2 |Y_p|^2 - \langle X_p, Y_p \rangle^2. \quad (2.5)$$

is the square of the area of the parallelogram generated by X_p and Y_p . It is well known that $k(P)$ depends only on the plane P , and not on the specific choice of X_p and Y_p .

In order to clarify the mentioned close relationship between the second fundamental tensor and the Hessian of real-valued functions, we recall first that for any field Z of normal vectors on M , the second fundamental form of M in the direction Z is the bilinear form

$$(X, Y) \rightarrow \langle \bar{\nabla}_X Z, Y \rangle \quad (2.6)$$

defined for arbitrary vector fields X and Y tangent to M . Because of

$\langle Z, Y \rangle = 0$, it follows that

$$0 = X \cdot \langle Z, Y \rangle = \langle \bar{\nabla}_X Z, Y \rangle + \langle Z, \bar{\nabla}_X Y \rangle = \langle \bar{\nabla}_X Z, Y \rangle + \langle V(X, Y), Z \rangle .$$

and hence that

$$\langle \bar{\nabla}_X Z, Y \rangle = -\langle V(X, Y), Z \rangle \quad (2.7)$$

Now, with fixed $p \in M$ and $Z_p \in N_p M$. consider the functional

$$\gamma : M \rightarrow \mathbb{R}, \quad \gamma(q) = \langle q - p, Z_p \rangle, \quad \text{for } q \in M. \quad (2.8)$$

It is a standard and elementary result that $d\gamma(p) = 0$; that is, that p is a critical point of γ . The Hessian of γ at p is then the bilinear form

$$H_\gamma(X_p, Y_p) = (X \cdot (Y \cdot \gamma))_p, \quad (2.9)$$

on $T_p M$, where X and Y are any vector fields tangent to M which coincide at p with X_p and Y_p , respectively. Let Z be a field of vectors normal to M such that Z coincides with Z_p at p . Then, at p , the second fundamental form of M in the direction Z is exactly the negative of the Hessian of γ at p (see e.g. [1, p.198]). In other words, (2.7) implies that

$$H_\gamma(X_p, Y_p) = \langle V(X_p, Y_p), Z_p \rangle, \quad (2.10)$$

In Section 5 this relation will provide the basis for the determination of bifurcation direction.

3. Properties of the second fundamental tensor.

Let X_p and Y_p be arbitrary vectors of $T_p M$ and suppose that $W_p = \alpha X_p + \beta Y_p$ with some real numbers $\alpha \neq 0$ and $\beta \neq 0$. The bilinearity and symmetry of the second fundamental tensor then implies that

$$V(X_p, Y_p) = \frac{1}{2\alpha\beta} [V(W_p, W_p) - \alpha^2 V(X_p, X_p) - \beta^2 V(Y_p, Y_p)] , \quad (3.1)$$

Observe that $V(X_p, Y_p)$ can be computed for arbitrary vectors X_p and Y_p of $T_p M$, if the $d(d+1)/2$ values $V(X_i, X_j)$, $1 \leq i \leq j \leq d$, are known for some basis $(X_i)_{i=1,d}$ of the tangent space $T_p M$. Moreover, because of (3.1), the computation of the quantities $V(X_i, X_j)$ can be reduced to that of the $d(d+1)/2$ terms $V(X_i, X_i)$, $1 \leq i \leq d$ and (say) $V(X_i + X_j, X_i + X_j)$, $1 \leq i < j \leq d$.

Our algorithm for the calculation of $V(X_p, Y_p)$, will be based on an elementary geometric construction. Suppose that $|X_p| = 1$ and introduce the space

$$\Pi = \text{span}(X_p) \oplus N_p M \subset \mathbb{R}^n . \quad (3.2)$$

Note that $\dim \Pi = n - d + 1$ and that, because of the (trivial) relation

$$\mathbb{R}^n = T_p M + \Pi ,$$

the affine space $p + \Pi$ intersects the manifold M transversally at p . Thus, locally near p , $(p + \Pi) \cap M$ is a curve C and

$$T_p C = \Pi \cap T_p M = \text{span}(X_p) .$$

Since $|X_p| = 1$, we can construct, locally near p , a field X of unit vectors tangent to M which along C is tangent to C and coincides at p with X_p . Indeed, we first define X along C through an arclength parametrization of that curve and then extend X to a neighborhood of C in M . Since, by construction, X is unit vector field on C , it is trivial that this extension may be chosen so that $|X| = 1$.

Because $C \subset p + \Pi$ and X is tangent to C along C , it follows that

$$\bar{\nabla}_X X \in \Pi \quad \text{along } C$$

and, in particular, that

$$(\bar{\nabla}_X X)_p \in \Pi . \quad (3.3)$$

Moreover, $|X| = 1$ implies that

$$0 = X \cdot 1 = X \cdot \langle X, X \rangle = 2 \langle \bar{\nabla}_X X, X \rangle ,$$

whence $(\bar{\nabla}_X X)_p$ is normal to X_p and together with (3.2) and (3.3) we obtain

$$(\bar{\nabla}_X X)_p \in N_p^M .$$

In other words, the tangential component of $\bar{\nabla}_X X$ vanishes at p so that in view of (2.1),

$$(\bar{\nabla}_X X)_p = V(X_p, X_p) . \quad (3.4)$$

On the other hand, because $|X| = 1$ and X is tangent to C along C , we have by definition

$$|(\bar{\nabla}_X X)_p| = k_p (\geq 0) , \quad (3.5)$$

where k_p is the curvature of C at p . Moreover, if $k_p \neq 0$, the principal normal n_p of length $|n_p| = 1$ is defined and

$$(\bar{\nabla}_X X)_p = k_p n_p , \quad (3.6)$$

Altogether, (3.4), (3.5) and (3.6) show that

$$\begin{aligned} V(X_p, X_p) &= 0 \text{ if } k_p = 0 , \\ V(X_p, X_p) &= k_p n_p \text{ if } k_p > 0 . \end{aligned} \quad (3.7)$$

When $k_p \neq 0$, the osculating plane to C at p is the plane

$$\text{span} \{X_p, n_p\} \in R^n .$$

A standard result of the local theory of curves states that the osculating plane is the limit of the planes $\text{span}(q_1-p, q_2-p)$ for any two distinct points $q_i \neq p$, $i=1,2$ of C that tend to p . Since $k_p \neq 0$ it follows that p and q_1, q_2 are not co-linear (see [12, Vol. II] for curves in R^3 ; the argument extends easily to curves in R^n). Thus q_1, q_2 and p define a circle in R^n and for

$q_i \rightarrow p, i=1,2$, the limit of these circles is a circle C in the osculating plane with radius

$$r_p = 1/k_p \quad (3.8)$$

This is the osculating circle at p .

4. A Computational Algorithm for the Fundamental Tensor

In general, whenever manifolds arise in numerical calculations, they are defined either through a local parametrization which is an immersion or, implicitly, as the zero set of a submersion. As in [8]-[10] it will suffice to consider only the latter case. Hence, suppose that $F: \Omega \subset \mathbb{R}^n \rightarrow \mathbb{R}^m$ is smooth on the open set Ω and $\text{rank } DF(q) = m$ for all $q \in \Omega$. We assume always that $d = n-m \geq 2$. Then

$$M = \{q \in \Omega ; F(q) = 0\} \quad (4.1)$$

is a d -dimensional submanifold of \mathbb{R}^n . For any $p \in M$ we identify the tangent space $T_p M$ with $\ker DF(p)$ and the normal space $N_p M$ with $(\ker DF(p))^\perp = \text{rge } DF(p)^*$ where as usual the asterisk denotes the adjoint operator. There are various possible methods for the computation of the orthonormal bases of $T_p M$ and $N_p M$; for instance, a simple approach is based on the use of the QR-factorization of $DF(p)^*$, (see also [10]).

For any given $X_p \in T_p M, X_p \neq 0$, and sufficiently small nonzero $h \in \mathbb{R}$ the implicit function theorem ensures the existence of a unique point $w(h) \in N_p M$ such that

$$F(p + hX_p + w(h)) = 0. \quad (4.2)$$

Once again, there are various methods for computing $w(h)$. In particular, if

the QR-factorization of $DF(p)^*$ is already available, a chord-Gauss-Newton process can be applied -- with $q = p + hX_p$ as starting point -- to project q onto M along $N_p M$. We refer to [10] for details and a convergence result. Note that the process of projecting q onto M requires only the evaluation and decomposition of the Jacobian of F at p . Of course, we may use other decompositions than the QR-factorization.

As in the previous section and with the notation (3.2), let $C = M \cap (p + \Pi)$ denote the curve induced on M by the given vector $X_p \in T_p M$. Then, for small $|h|$ we have $p + hX_p + w(h) \in M \cap (p + \Pi) = C$. This suggests that we compute for some $h > 0$ the points

$$q_1 = p + hX_p + w(h), \quad q_2 = p + hX_p + w(-h)$$

on M . Then, if $k_p \neq 0$ and h is sufficiently small, the triangle formed by q_1 , q_2 , and p in the plane $\text{span}(q_1 - p, q_2 - p)$ is not degenerate.

The well-known Heron formula of planar geometry states that for a non-degenerate triangle with side lengths a, b, c , the curvature \bar{k} of the circumscribing circle is given by

$$\bar{k} = \frac{4}{abc} [s(s-a)(s-b)(s-c)]^{1/2} \quad (4.3)$$

where $s = (a+b+c)/2$. In our case, the sides $a = |q_1 - p|$ and $b = |q_2 - p|$ are equal up to order h^2 and the third side is almost equal to their sum. Hence it is natural to introduce the scaled quantities $a_c = a/c$, and $b_c = b/c$, and to rewrite (4.3) in the form

$$\bar{k} = \left(\frac{1}{c}\right) \left[\frac{1}{a_c} + \frac{1}{b_c}\right] (1 - \delta^2)^{1/2} (1 - \gamma^2)^{1/2} \quad (4.4)$$

where $\delta = a_c - b_c$ and $\gamma = 1/(a_c + b_c)$. The term in square brackets is close to 4 while the first square root is approximately equal to one. Thus, both of these terms can be evaluated safely. But, in the last square root γ is close

to one, and hence we compute that term as

$$\phi = \arcsin(\gamma), \quad (1 - \gamma^2)^{1/2} = \cos(\phi) \quad (4.5)$$

When $1 - \gamma$ falls below machine precision then, in floating point arithmetic, ϕ will be zero and we set $\bar{k} = 0$.

Clearly, when h tends to zero then the circle through the points q_i , $i=1,2$ and p tends to the osculating circle and hence \bar{k} becomes the curvature k_p of the curve C at p . Thus our algorithm produces an approximation \bar{k} of k_p .

If \bar{k} is not zero, then an approximation \bar{n} of the normal vector n_p can be generated by orthogonalizing the vector $v = (q_1 - p) + (q_2 - p)$ with respect to X_p and then normalizing the result to length one; that is, by applying the algorithm

$$\bar{n} := v - \langle X_p, v \rangle X_p, \quad \bar{n} := \frac{\bar{n}}{|\bar{n}|}$$

Thus altogether, we have obtained an approximation $\bar{V}(X_p, X_p) = \bar{k} \bar{n}$ of $V(X_p, X_p)$.

As noted in the previous section, the calculation of the fundamental tensor V can be reduced to the computation of the $d(d+1)/2$ quantities $V(X_i, X_i)$, $1 \leq i \leq d$ and $V(X_i + X_j, X_i + X_j)$, $1 \leq i < j \leq d$ for some basis X_i , $i = 1, \dots, d$ of $T_p M$. Of course, this basis may be chosen in various ways; we indicate here only some advantageous choices in the cases $d = 2, 3$. For this purpose, suppose that an orthogonal basis of $T_p M$ is already available which then defines an isomorphism U from \mathbb{R}^d onto $T_p M$.

For $d = 2$ we introduce in \mathbb{R}^2 the vectors

$$X_1 = U \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad X_2 = \frac{1}{2} U \begin{pmatrix} -1 \\ r \end{pmatrix}, \quad X_3 = X_1 + X_2$$

where, for ease of notation, $r = 3^{\frac{1}{2}}$. Then, with the above algorithm, the values $V_i = V(X_i, X_i)$, $i = 1, 2, 3$, of the second fundamental tensor can be computed, and, by (3.1), we obtain

$$V_{12} = V(X_1, X_2) = \frac{1}{2}(V_1 + V_2 - V_3).$$

Now for any two vectors $Y_1, Y_2 \in T_p M$ it follows that

$$Y_i = \alpha_i X_1 + \beta_i X_2, \quad i = 1, 2$$

with

$$\begin{pmatrix} \alpha_i \\ \beta_i \end{pmatrix} = \frac{2}{3} \begin{pmatrix} 2 & 1 \\ 1 & 2 \end{pmatrix} \begin{pmatrix} Y_i^T X_1 \\ Y_i^T X_2 \end{pmatrix}, \quad i = 1, 2$$

and hence that

$$V(Y_1, Y_2) = \alpha_1 \alpha_2 V_1 + (\alpha_1 \beta_2 + \alpha_2 \beta_1) V_{12} + \beta_1 \beta_2 V_2. \quad (4.6)$$

For $d = 3$ we proceed analogously and introduce the vectors

$$X_1 = U \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, \quad X_2 = \frac{1}{2} U \begin{pmatrix} -1 \\ r \\ 0 \end{pmatrix}, \quad X_3 = \frac{1}{4} U \begin{pmatrix} -1 \\ -r \\ 2r \end{pmatrix}$$

and

$$X_4 = X_1 + X_2, \quad X_5 = \left(\frac{2}{3}\right)^{\frac{1}{2}}(X_1 + X_3), \quad X_6 = \left(\frac{2}{3}\right)^{\frac{1}{2}}(X_2 + X_3)$$

Then, once again, we compute $V_i = V(X_i, X_i)$, $i = 1, \dots, 6$, and

$$V(X_1, X_2) = V_{12} = \frac{1}{2}(V_4 - V_1 - V_2),$$

$$V(X_1, X_3) = V_{13} = \frac{3}{4}V_5 - \frac{1}{2}(V_1 + V_3),$$

$$V(X_2, X_3) = V_{23} = \frac{3}{4}V_6 - \frac{1}{2}(V_2 + V_3).$$

Now for any three vectors $Y_i \in T_p M$, $i = 1, 2, 3$, we have

$$Y_i = \alpha_i X_1 + \beta_i X_2 + \gamma_i X_3, \quad i = 1, 2, 3$$

with

$$\begin{pmatrix} \alpha_i \\ \beta_i \\ \gamma_i \end{pmatrix} = \frac{1}{3} \begin{pmatrix} 5 & 3 & 2 \\ 3 & 5 & 2 \\ 2 & 2 & 4 \end{pmatrix} \begin{pmatrix} Y_i^T X_1 \\ Y_i^T X_2 \\ Y_i^T X_3 \end{pmatrix}, \quad i = 1, 2, 3$$

and hence

$$\begin{aligned} V(Y_1, Y_2) &= \alpha_1 \alpha_2 V_1 + \beta_1 \beta_2 V_2 + \gamma_1 \gamma_2 V_3 \\ &+ (\alpha_1 \beta_2 + \alpha_2 \beta_1) V_{12} + (\beta_1 \gamma_2 + \beta_2 \gamma_1) V_{23} + (\alpha_1 \gamma_2 + \alpha_2 \gamma_1) V_{13}. \end{aligned}$$

It should be evident how we might proceed for higher dimensional manifolds M . Note that, independent of the dimension d of M , the computation of the fundamental tensor at a point p of M requires only one evaluation and decomposition of the Jacobian of F , namely at p . The computational cost for this is of order n^3 , where, of course, n is the dimension of the embedding space. Once the decomposed Jacobian at p is available, the cost of projecting each one of the $d(d+1)$ required points onto M is of order n^2 while all other parts of the algorithms involve a lower order of operations.

5. Determination of Bifurcation Directions

As in section 4, suppose again that the smooth mapping $F: \Omega \subset \mathbb{R}^n \rightarrow \mathbb{R}^m$, ($d = n - m \geq 2$) satisfies $\text{rank } DF(q) = m$ for all q on the open set Ω and hence that (4.1) defines a d -dimensional submanifold of \mathbb{R}^n . At a given point $p \in M$, we consider, as in [8], local coordinate systems which are induced by some d -

dimensional linear subspace T of R^n . More specifically, if $T \cap N_p M = \{0\}$ then it follows from the implicit function theorem that there exist open neighborhoods $Q \subset T$ of the origin of T , and $S \subset R^n$ of p , respectively, and a smooth mapping $f: Q \rightarrow T^\perp$ such that $f(0) = 0$ and $M \cap S = \theta(Q)$ where

$$\theta: Q \rightarrow R^n, \quad \theta(u) = p + u + f(u) \in R^n, \quad u \in Q. \quad (5.1)$$

Note that always $D\theta(0)u \in T_p M$ for $u \in Q$ and hence that for the local coordinate system induced by $T = T_p M$ we have $Df(0) = 0$. For this case we consider here the numerical evaluation of the bilinear mapping

$$(X_p, Y_p) \in T_p M \times T_p M \rightarrow D^2 f(0)(X_p, Y_p). \quad (5.2)$$

Let Z_1, \dots, Z_m be an orthonormal basis of the normal space $N_p M$ and hence

$$f = f_1 Z_1 + \dots + f_m Z_m, \quad f_i = \langle f, Z_i \rangle, \quad i=1, \dots, m. \quad (5.3)$$

For each Z_i , $1 \leq i \leq m$, we consider, as in (2.8), the functional

$$\gamma_i: M \rightarrow R, \quad \gamma_i(q) = \langle q - p, Z_i \rangle, \quad \text{for } q \in M \quad (5.4)$$

for which

$$\gamma_i(q) = \langle u + f(u), Z_i \rangle = \langle f(u), Z_i \rangle = f_i(u), \quad \text{for } q \in Q, \quad (5.5)$$

and hence $f_i = \gamma_i \circ \theta$. Since, $Df(0) = 0$ we have $D\gamma_i(0) = 0$ and $D\theta(0)X_p = X_p$ for any $X_p \in T_p M$. Thus the Hessian H_i of γ_i at p is given by

$$H_i(X_p, Y_p) = D^2 f_i(0)(X_p, Y_p), \quad \text{for all } X_p, Y_p \in T_p M.$$

Now (2.10) implies that

$$D^2 f_i(0)(X_p, Y_p) = \langle V(X_p, Y_p), Z_i \rangle, \quad i=1, \dots, m, \quad (5.6)$$

whence, by (5.3),

$$D^2 f(0)(X_p, Y_p) = V(X_p, Y_p).$$

In other words, the second fundamental tensor of M at p is exactly the second

derivative of f at the origin of $T_p M$. Note that this simple relation is valid only when $Df(0) = 0$; that is, when the local coordinate system at p is induced by the tangent space. But that is a natural choice in the framework of bifurcation problems.

Generally, in applications a d -dimensional natural parameter subspace $\Lambda \subset \mathbb{R}^n$ is identified. We follow here the approach in [4] and call a point $p \in M$ a foldpoint (with respect to Λ) if Λ does not induce a local coordinate system at p ; that is, if

$$N_0 = \Lambda \cap N_p M \neq \{0\}.$$

The integer $r_1 = \dim(N_0)$ is the first singularity index of the foldpoint and the set

$$\{q \in M; \langle q - p, n \rangle = 0, \text{ for all } n \in N_0\}$$

the cutset of M at p . Let $Z_i, i=1, \dots, r_1$ be an orthonormal basis of N_0 and extend it to an orthonormal basis of all of $N_p M$. Then it follows from (5.4) and (5.5) that, locally near p , the cutset is the zero set of the mapping

$$g: Q \subset T_p M \rightarrow \mathbb{R}^{r_1}, \quad g(u) = (f_1(u), \dots, f_{r_1}(u))^T, \quad u \in Q. \quad (5.7)$$

Evidently, we have $g(0) = 0$, $Dg(0) = 0$, and if $r_2 \geq 1$ exists such that

$$D^k g(0) = 0, \quad k=0, 1, \dots, r_2, \quad D^{r_2+1} g(0) \neq 0$$

then r_2 is called the second singularity index of p . Under some non-degeneracy conditions (see e.g. [2], [4], or [6]), the form of the cutset is determined, locally near p , by the nontrivial zeroes of the (r_2+1) -form

$$D^{r_2+1} g(0)(X_p, \dots, X_p), \quad X_p \in T_p M.$$

For $r_2 = 1$ it follows from (5.7) that

$$D^2g(0)(X_p, X_p) = (\langle V(X_p, X_p), Z_1 \rangle, \dots, \langle V(X_p, X_p), Z_{r_1} \rangle), \quad X_p \in T_p M. \quad (5.8)$$

In other words, the bifurcation directions at p are the zeroes $X_p \in T_p M$, $X_p \neq 0$ of the r_1 quadratic equations

$$\langle V(X_p, X_p), Z_i \rangle = 0, \quad i=1, \dots, r_1. \quad (5.9)$$

It may be useful to reformulate this result for the standard setting of bifurcation theory. For this suppose that $G: R^m \times R^1 \rightarrow R^m$ is a smooth mapping on some open neighborhood of a point $(\bar{y}, \bar{\lambda}) \in R^m \times R^1$ where $G(\bar{y}, \bar{\lambda}) = 0$ and $\dim \ker DG(\bar{y}, \bar{\lambda}) = r+1 \geq 2$. For ease of notation we shall write here also $x = (y, \lambda)$ and, in particular, $\bar{x} = (\bar{y}, \bar{\lambda})$. Note that the conditions on G imply that $\dim \ker D_y G(\bar{x}) = r \geq 1$ and $\dim \text{rge } DG(\bar{x}) = m-r \leq m-1$. Let $a_1, \dots, a_r \in R^m$ be linearly independent vectors which span $\ker DG(\bar{x})^*$. Then $\text{span}(a_1, \dots, a_r)$ is a complement of $\text{rge } DG(\bar{x})$ in R^m which suggests the introduction of the unfolding

$$F: R^m \times \Lambda \rightarrow R^r, \quad \Lambda = R^1 \times R^m, \quad F(y, \lambda, \delta) = G(y, \lambda) + \delta_1 a_1 + \dots + \delta_r a_r \quad (5.10)$$

where $\delta = (\delta_1, \dots, \delta_r)$. With $n=m+1+r$, $d=r+1$, $q = (y, \lambda, \delta)$ this corresponds exactly to the earlier setting. Clearly, we have $F(p) = 0$ at $p = (\bar{x}, 0)$ and the condition $\text{rge } DF(p) = m$ holds in an open neighborhood of p . Hence the d -dimensional manifold (4.1) is well-defined and p is a foldpoint with respect to Λ with first singularity index $r_1 = r$. Since

$$DF(p)^* a_i = e_{n-r+i}, \quad i=1, \dots, r$$

where e_j are the natural basis vectors of R^n , the set $N_0 = \Lambda \cap N_p M$ is spanned here by $Z_i = e_{n-r+i}$, $i=1, \dots, r$ and the cutset is the solution set of the equations $F = 0$, $\delta = 0$ and hence of $G = 0$. Our local coordinate system is given now by

$$\theta(\xi) = (x + \xi, \delta(\xi)), \quad \xi \in \ker DG(\bar{x})$$

Thus we have $f_i = \langle \delta, e_{n-r+i} \rangle = \delta_i$, $i=1, \dots, r$ and (5.6) becomes

$$D^2\delta_i(0)(\xi, \eta) = \langle V((\xi, 0), (\eta, 0)), Z_i \rangle, \quad i=1, \dots, r, \text{ for } \xi, \eta \in \ker DG(\bar{x}).$$

Hence, if the foldpoint has second singularity index $r_2 = 1$, then under the mentioned non-degeneracy condition the bifurcation directions for $G = 0$ are exactly the solutions of the quadratic equation

$$D^2\delta(0)(\xi, \xi) = 0 \quad (5.11)$$

In bifurcation theory, the characterization of the bifurcation directions, given here in terms of δ , is usually formulated in terms of the reduced mapping obtained after transforming the equation $G = 0$ by means of the Lyapunov-Schmidt reduction. While both characterizations give equivalent results, the method we use here completely bypasses the Lyapunov-Schmidt reduction and allows for all calculations to be performed in the framework of the smooth manifold (4.1) on which no singularity hampers the computations.

The equations (5.9) (or (5.11)) determining the bifurcation directions are readily solvable. In fact, suppose, as in section 4, that X_1, \dots, X_d is a basis of $T_p M$ for which the components $V_{ij} = V(X_i, X_j)$, $1 \leq i \leq j \leq d$ of the second fundamental tensor have been computed. Then (5.9) reduces to a system of homogeneous quadratic equations

$$x^T A_k x = 0, \quad x \in \mathbb{R}^d, \quad x \neq 0 \quad (5.12)$$

where the $d \times d$ -matrices A_k have the elements

$$a_{ij}^k = \langle V_{ij}, Z_k \rangle, \quad 1 \leq i, j \leq d, \quad k = 1, \dots, r_1$$

and

$$X_p = x_1 X_1 + \dots + x_d X_d.$$

This system of quadratic equations can have finitely many isolated solutions

only in the case $d = r_1 + 1$. Hence this is the only case for which solutions will be sought numerically. Clearly, for small d the system is easily solvable. The case $d = 2$, ($r_1 = 1$) is, of course trivial, and also for the case $d = 3$, ($r_1 = 2$) simple methods are available. In fact, (5.12) has non-trivial solutions only when all matrices are indefinite. Thus in the (3x3)-case each A_k must have one eigenvalue of different sign than the other two. Hence, if there is no degeneracy, then, after diagonalization, the first of the two equations has the form

$$\mu_1 \xi_1^2 = \mu_2 \xi_2^2 + \mu_3 \xi_3^2$$

with $\mu_i > 0$, $i=1,2,3$. This suggests the normalization $\xi_1 = 1$ and the use of the elliptic coordinates $\xi_2 = \alpha \cos(\tau)$, $\xi_3 = \beta \sin(\tau)$, $0 \leq \tau \leq \pi$ where $\alpha = (\mu_1/\mu_2)^{1/2}$, $\beta = (\mu_1/\mu_3)^{1/2}$. Now we can readily detect the intervals in the τ -variable on which the corresponding residual of the second equation changes sign, which, in turn, allows the application of a standard root finder for determining the solutions.

Clearly, for larger dimensions such simple approaches are not readily available, and the system (5.12) has to be solved by means of one of the polynomial root finders as, for example, the CONSOL system, [5].

6. Numerical Examples

In order to demonstrate the performance of the algorithm, we present here some numerical results obtained with a FORTRAN implementation run in double precision on a VAX-cluster.

As a first, very simple problem, consider the cusp

$$F: \mathbb{R}^3 \rightarrow \mathbb{R}^1, \quad F(x) = x_1^3 - x_1 x_2 - x_3, \quad \text{for } x \in \mathbb{R}^3. \quad (6.1)$$

The tangent space at $x = 0$ is $T_x M = \text{span}(e_1, e_2)$ where $e_i, i=1,2,3$ are the natural basis vectors of \mathbb{R}^3 . A straightforward calculation shows that at $x = 0$ we have

$$V(u_1, u_2) = -\sin(\phi_1 + \phi_2)e_3, \quad \text{for } u_i = (\cos(\phi_i), \sin(\phi_i), 0)^T \in T_x M, \quad i=1,2. \quad (6.2)$$

Table 1 gives some comparison of computed values of the curvature and their corresponding exact values $k_x = |\sin(\phi_1 + \phi_2)|$ for different choices of the two angles. Here we used a step $h = 0.005$ in the curvature evaluations and a tolerance of 10^{-6} for the projection of the points onto the manifold.

Table 1: Curvature of the Cusp Function			
ϕ_1	ϕ_2	Exact	Computed
0	0	0.0	0.0
0	0.3π	0.809017	0.809013
0	0.6π	0.951057	0.951052
0	0.9π	0.309017	0.309016
0.3π	0.3π	0.951057	0.951052
0.3π	0.4π	0.809017	0.809013
0.3π	0.5π	0.587785	0.587782
0.6π	0.6π	0.587785	0.587782
0.6π	0.9π	1.0	0.999995
0.8π	0.9π	0.809017	0.809013

The computed values certainly are in excellent agreement with the exact data. All our experience so far indicates that the curvature algorithm is indeed very reliable, not just for small problems as this one.

As a second example, consider the two point boundary value problem

$$-u'' - \lambda u + \alpha u^2 = 0, \quad u(0) = u(\pi) = 0 \quad (6.3)$$

which, after a straightforward discretization and in unfolded form, leads to the finite dimensional system

$$Ay + h^2(\alpha Q(y) - \lambda y) + \mu w = 0, \quad y \in \mathbb{R}^k, \quad h = \pi/(k+1). \quad (6.4)$$

Here $Q(y) = (y_1^2, \dots, y_k^2)^T$ and A is the symmetric, tri-diagonal, $k \times k$ matrix with diagonal elements 2 and sub-diagonal entries -1 . Thus, with $q = (y, \lambda, \mu) \in \mathbb{R}^n$ and $n = k+2$, $m = k$, $d = 2$, (6.4) is a problem of the form considered in sections 4 and 5.

Let $\sigma_1 < \dots < \sigma_k$ be the eigenvalues of A . The unfolding vector w was chosen as a normalized eigenvector of A corresponding to the eigenvalue σ_i for a given i . Then $p = (0, \sigma_i/h^2, 0)$ is a foldpoint of (6.4) with respect to the parameter space spanned by the basis vectors e_{n-1}, e_n of \mathbb{R}^n and both singularity indices of p equal one. A theoretical analysis of (6.3) shows that each p is a bifurcation point and that for odd values of i the bifurcation is transcritical while for even i the branches intersect at a right angle. More specifically, for odd i the angle α_i between the bifurcating branches satisfies

$$\gamma_i = \cos(\alpha_i) = \tau / (1 + \tau^2)^{1/2}, \quad \tau = w_1^3 + \dots + w_k^3 \quad (6.5)$$

where w_1, \dots, w_k are the components of w .

Table 2 shows the computed and theoretical values of γ_i for $i = 1, \dots, k$ in the case $k = 15$. Again the agreement between the computed and the predicted data is excellent.

Table 2: γ_i -values (6.5)		
i	Exact	Computed
1	0.287444	0.287445
2	0.0	0.155(-15)
3	0.996991	0.996700
4	0.0	0.673(-16)
5	0.608096(-1)	0.608102(-1)
6	0.0	0.0
7	0.462437(-1)	0.462441(-1)
8	0.0	0.171(-11)
9	0.478171(-1)	0.478175(-1)
10	0.0	0.160(-15)
11	0.940416(-1)	0.940424(-1)
12	0.0	0.801(-17)
13	0.340802(-2)	0.340805(-2)
14	0.0	0.171(-11)
15	0.869785(-4)	0.869794(-4)

As a third problem we consider the discrete Brusselator (see e.g. [7]) in unfolded form

$$\begin{aligned}
 Ay - \lambda h^2((\beta-1)y + 9z + G(y,z,\beta)) + \mu w_1 &= 0 \\
 Ay + 0.25\lambda h^2(\beta y + 9z + G(y,z,\beta)) + \nu w_2 &= 0
 \end{aligned}
 \quad h = \pi/(k+1), \quad y, z \in \mathbb{R}^k \quad (6.5)$$

where again A is the tri-diagonal, $k \times k$ matrix used in (6.4), and

$$G(y,z,\beta) = (g(y_1, z_1, \beta), \dots, g(y_k, z_k, \beta))^T, \quad g(s, t, \beta) = (\frac{1}{3}\beta + t)s^2 + 6st$$

With $q = (y, z, \lambda, \mu, \nu) \in \mathbb{R}^n$ and $n = 2k+3$, $m = 2k$, $d = 3$ this is a problem of the form considered in sections 4 and 5. If again $\sigma_1 < \dots < \sigma_k$ are the eigenvalues of A then some calculation shows that $p = (0, 0, \lambda, 0, 0)$ with

$$\lambda = \frac{2}{3h^2} (\sigma_1 \sigma_j)^{\frac{1}{2}}, \quad \beta = \frac{13}{4} + \frac{3}{2} \frac{\sigma_1 + \sigma_j}{(\sigma_1 \sigma_j)^{\frac{1}{2}}}, \quad i \neq j \quad (6.6)$$

is a foldpoint of (6.5) with respect to the parameters λ, μ, ν and with first and second singularity indices 2 and 1, respectively. For $k = 3$ and $i = 1, j = 2$, (6.6) gives the values $\lambda = 1.08158$, $\beta = 6.83343$ used in [7], while for $k = 8$ they become $\lambda = 1.14009$, $\beta = 6.96599$. In each case, our algorithm determined four bifurcation directions. For $k = 3$ the computed directions are given in Table 3. This appears to be the first computational determination of bifurcation directions for singularities with co-dimension larger than 2 in the literature.

Table 3: Bifurcation Directions for the Brusselator			
#1	#2	#3	#4
-0.646189(-6)	0.777229	0.253517	-0.380313
-0.594689(-6)	0.370361	-0.370326	-0.537862
-0.194827(-6)	-0.253460	-0.777237	-0.380338
-0.311403(-6)	-0.321441	-0.292234(-1)	0.212202
-0.331812(-6)	-0.206646	0.206627	0.300105
-0.157850(-6)	0.291988(-1)	0.321438	0.212211
-1.000000	0.218236	-0.218217	-0.491205
0.0	0.0	0.0	0.0
0.0	0.0	0.0	0.0

Clearly, once the bifurcation directions are available, a standard continuation process (see e.g. [11]) can be started to follow the corresponding solution branch.

The examples certainly indicate that the algorithms presented here perform very well in practice. As noted, our experience has shown that the curvature computations are very reliable. Of course, in the above examples we

always worked with an exactly known foldpoint p with known singularity indices. In practice, one often has only some approximation of such a point. But in our approach, this is not a serious concern. In fact, the second fundamental tensor V is a smooth function of the base point on the manifold M and hence the computed V can be expected to be an approximation of V at the exact foldpoint. Thus for any chosen normal vectors Z_i the quadratic equations (5.9) should also be close to the corresponding equations at p itself. This leaves only the determination of the critical first singularity index r_1 and of the normal vectors Z_i that span the intersection $\Lambda \cap N_p M$. We refer to [7] for some comments about the determination of r_1 , and to [3] for a method to compute an approximation of the basis vector in the case $r_1 = 1$.

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